APPENDIX 2
Table 8

Dimit Atom	Amino Acid in full length α	Amino Acid Atom	Distance A
C16	215-PHE	CD1	3.98
C16	215-PHE	CE1	3.86
C19	218-PHE	O	3.69
C16	218-PHE	CB	3.89
C18	218-PHE	CB	3.92
C19	218-PHE	CB	4.13
C18	218-PHE	CD2	3.77
C16	219-THR	CG2	3.68
C19	221-ILE	CG1	4.11
C6	222-ILE	CD1	4.18
C8	222-ILE	CD1	3.72
C10	222-ILE	CD1	3.53
C12	222-ILE	CD1	3.85
O1	222-ILE	CD1	4.13
C13	225-ALA	C8	3.64
O4	225-ALA	C8	4.02
O4	228-ARG	CZ	3.96
C17	228-ARG	NH2	3.36
O3	228-ARG	NH2	3.58
O4	228-ARG	NH2	2.86
C10	256-MET	SD	3.70
C12	256-MET	SD	3.89
C10	256-MET	CE	3.88
C12	256-MET	CE	3.83
C11	259-MET	C	4.03
C11	259-MET	O	3.66
C15	259-MET	O	3.42
N1	259-MET	O	3.71
C1	259-MET	C8	4.20
C11	259-MET	C8	3.87
C13	259-MET	C8	4.09
C15	262-ARG	C8	4.03
C17	262-ARG	C8	3.58
O3	262-ARG	C8	3.62
O4	262-ARG	C8	3.85
C17	262-ARG	CD	4.10
O4	262-ARG	CD	3.61
N1	263-ALA	N	3.71
C17	263-ALA	CA	3.69
N1	263-ALA	CB	3.46
O3	266-ARG	NH1	3.93
N1	275-THR	O	3.62
N1	276-LEU	CA	3.51
N1	276-LEU	C	3.92
C5	276-LEU	CD1	4.05
C19	276-LEU	CD1	4.04
C7	276-LEU	CD2	4.09
C9	276-LEU	CD2	3.95
C11	276-LEU	CD2	4.13
N1	276-LEU	CD2	4.17
C13	277-SER	N	4.14
C15	277-SER	N	3.79

Dimit Atom	Amino Acid in full length α	Atom	Distance A
C17	277-SER	N	3.69
N1	277-SER	N	3.30
O3	277-SER	N	3.19
C17	277-SER	CA	3.92
O3	277-SER	CA	3.35
C13	277-SER	OG	3.92
C7	287-LEU	CD2	3.90
C18	290-GLY	C	4.04
C18	290-GLY	O	3.54
C18	291-GLY	CA	4.04
C18	292-LEU	N	4.20
C2	292-LEU	CG	4.18
C4	292-LEU	CG	3.86
C6	292-LEU	CG	4.01
C2	292-LEU	CD1	3.88
C4	292-LEU	CD1	4.02
O2	292-LEU	CD1	4.07
C4	292-LEU	CD2	4.05
C6	292-LEU	CD2	3.72
C8	292-LEU	CD2	3.69
C10	292-LEU	CD2	3.98
O1	292-LEU	CD2	4.16
C20	299-ILE	CD1	3.87
C8	381-HIS	CD2	3.90
C10	381-HIS	CD2	3.84
O1	381-HIS	GO2	3.40
O1	381-HIS	CE1	3.72
C8	381-HIS	NE2	3.47
C10	381-HIS	NE2	3.51
O1	381-HIS	NE2	2.64
C6	388-MET	CE	3.90
C8	401-PHE	CE1	4.19
O1	401-PHE	CE1	3.37
C16	401-PHE	CZ	3.97
O1	401-PHE	CZ	3.28
N1	502-H_2O	O1	3.35
O3	502-H_2O	O1	2.56
O3	503-H_2O	O1	3.13
O4	503-H_2O	O1	3.72
O4	504-H_2O	O1	2.72

Legend to Table 8. The table lists the interactions with Dimit (DMT). The column headings are as follows:

#1 The atom of Dimit that interacts with the amino acid of the receptor. These are also numbered in figure 32.

#2 The amino acid in the full length rTRα that interacts with the ligand.

#3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.

#4 The distance in A between Dimit and the protein atom.

Table 9

Triac Atom	Amino Acid in full length α	Amino Acid Atom	Distance A
I1	218-PHE	O	3.52
I1	221-ILE	CD1	4.16
I1	221-ILE	CG1	3.92
I1	222-ILE	CA	4.15
I1	222-ILE	CB	4.03
I1	222-ILE	CG1	3.92
C8	222-ILE	CD1	4.12
C10	222-ILE	CD1	3.77
C12	222-ILE	CD1	3.79
C13	225-ALA	CB	4.17
C3	225-ALA	CB	3.86
C10	256-MET	SD	3.45
C12	256-MET	SD	3.73
C10	256-MET	CE	3.66
C12	256-MET	CE	3.77
I3	256-MET	CE	3.89
C1	259-MET	O	3.93
C11	259-MET	O	3.24
O3	259-MET	O	4.09
C1	259-MET	CB	3.89
C13	259-MET	O	3.74
C14	259-MET	O	3.96
C1	259-MET	CB	3.89
C11	259-MET	CB	3.68
C13	259-MET	CB	4.01
C11	259-MET	CA	4.13
C13	259-MET	CA	4.20
I3	260-SER	CA	4.10
I3	260-SER	OG	4.19
C14	262-ARG	CB	4.07
O4	262-ARG	CB	3.60
O3	263-ALA	N	3.79
C14	263-ALA	N	4.12
O3	263-ALA	CA	3.67
O3	263-ALA	CB	3.49
C11	263-ALA	CB	4.00
C14	266-ARG	CZ	3.89
O3	266-ARG	CZ	4.01
O4	266-ARG	CZ	3.03
C14	266-ARG	NH1	3.25
O3	266-ARG	NH1	3.00
O4	266-ARG	NH1	2.82
C14	266-ARG	NH2	3.48
O3	266-ARG	NH2	4.01
O4	266-ARG	NH2	2.34
O3	275-THR	C	4.02
C14	275-THR	O	4.20
O3	275-THR	O	3.20
O3	278-LEU	CA	3.11
O3	276-LEU	C	3.52
O3	276-LEU	N	4.04
C14	276-LEU	CA	3.98
O3	276-LEU	CA	3.11

Triac Atom	Amino Acid in full length α	Amino Acid Atom	Distance A
C14	276-LEU	C	3.98
O3	276-LEU	CB	3.95
O2	276-LEU	CD1	4.03
I1	276-LEU	CD1	4.10
C7	276-LEU	CD2	3.84
C9	276-LEU	CD2	3.73
CII	276-LEU	CD2	4.06
O2	276-LEU	CD2	4.10
O3	276-LEU	CD2	3.91
C13	277-SER	N	4.06
C14	277-SER	N	3.13
O4	277-SER	N	3.28
O3	277-SER	N	3.05
C14	277-SER	CA	3.76
O4	277-SER	CA	3.52
C3	277-SER	OG	3.87
C13	277-SER	OG	4.02
C14	277-SER	OG	4.14
I2	290-GLY	O	3.57
I2	292-LEU	CG	3.94
C4	292-LEU	CG	3.95
C6	292-LEU	CG	3.65
C8	292-LEU	CG	4.02
C2	292-LEU	CD1	4.11
C4	292-LEU	CD1	3.85
C6	292-LEU	CD1	4.02
I2	292-LEU	CD2	3.98
C4	292-LEU	CD2	4.11
C6	292-LEU	CD2	3.44
C8	292-LEU	CD2	3.28
C10	292-LEU	CD2	3.88
O1	292-LEU	CD2	3.35
I3	299-ILE	CD1	3.77
C8	381-HIS	CD2	3.87
C10	381-HIS	CD2	3.90
O1	381-HIS	GO2	3.20
O1	381-HIS	CE1	3.82
C8	381-HIS	NE2	3.57
C10	381-HIS	NE2	3.52
O1	381-HIS	NE2	2.64
O1	388-MET	CE	4.03
O1	401-PHE	CE1	3.86
01	401-PHE	CZ	3.70
C13	460-H_2O	01	4.00

Legend to Table 9. The table lists the interactions with Triac. The column headings are as follows:
#1 The atom of Triac that interacts with the amino acid of the receptor. These are also numbered in figure 32.
#2 The amino acid in the full length rTRα that interacts with the ligand.
#3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.
#4 The distance in A between Triac and the protein atom.

Table 10

$lpBR_2$ Atom	Amino Acid in full length α	Amino Acid Atom	Distance A
C16	215-PHE	CD1	4.01
C16	215-PHE	CE1	3.78
BR1	218-PHE	O	3.24
BR1	218-PHE	C	3.98
C16	218-PHE	CB	3.81
C18	218-PHE	CB	3.92
BR1	218-PHE	CB	4.08
C18	218-PHE	CD2	3.92
C16	219-THR	CG2	3.45
BR1	221-ILE	CG1	3.81
BR1	221-ILE	CD1	4.07
BR1	222-ILE	CB	3.81
BR1	222-ILE	CG1	3.97
C6	222-ILE	CD1	4.07
C8	222-ILE	CD1	3.64
C10	222-ILE	CD1	3.50
C12	222-ILE	CD1	3.82
O1	222-ILE	CD1	4.08
C13	225-ALA	CB	3.76
O4	225-ALA	CB	4.01
O4	228-ARG	CZ	3.92
C17	228-ARG	NH2	3.26
O3	228-ARG	NH2	3.43
O4	228-ARG	NH2	2.79
C10	256-MET	SD	3.65
C12	256-MET	SD	3.71
C10	256-MET	CE	3.90
C12	256-MET	CE	3.75
BR2	256-MET	CE	4.03
C11	259-MET	C	3.98
C11	259-MET	O	3.52
C15	259-MET	O	3.44
N1	259-MET	O	3.76
C11	259-MET	CB	3.87
N1	262-ARG	C	4.03
C15	262-ARG	CB	4.03
C17	262-ARG	CB	3.56
O3	262-ARG	CB	3.55
O4	262-ARG	CB	3.91
C17	262-ARG	CD	4.09
O4	262-ARG	CD	3.71
N1	263-ALA	N	3.61
N1	263-ALA	CA	3.59
N1	263-ALA	CB	3.54
O3	266-ARG	NH1	3.93
N1	275-THR	O	3.43
N1	276-LEU	CA	3.46
N1	276-LEU	C	3.83
C5	276-LEU	CD1	4.02
C7	276-LEU	CD2	4.00
C9	276-LEU	CD2	3.81
C11	276-LEU	CD2	3.91
C13	277-SER	N	3.79

$IpBR_2$ Atom	Amino Acid in full length α	Amino Acid Atom	Distance A
C15	277-SER	N	3.63
C17	277-SER	N	3.70
N1	277-SER	N	3.17
03	277-SER	N	3.37
C17	277-SER	CA	3.89
03	277-SER	CA	3.43
C13	277-SER	OG	3.66
02	287-LEU	CD1	4.05
C18	290-GLY	C	4.04
C18	290-GLY	O	3.48
C18	291-GLY	CA	4.02
C4	292-LEU	CG	3.89
C6	292-LEU	CG	4.02
C2	292-LEU	CD1	3.79
C4	292-LEU	CD1	3.96
02	292-LEU	CD1	3.97
C4	292-LEU	CD2	4.07
C6	292-LEU	CD2	3.75
C8	292-LEU	CD2	3.67
C10	292-LEU	CD2	3.92
BR2	299-ILE	CD1	3.68
C8	381-HIS	CD2	3.92
C10	381-HIS	CD2	3.78
01	381-HIS	GD2	3.50
01	381-HIS	CE1	3.62
C8	381-HIS	NE2	3.36
C10	381-HIS	NE2	3.34
01	381-HIS	NE2	2.62
C8	401-PHE	CE1	4.02
01	401-PHE	CE1	3.19
C16	401-PHE	CZ	4.03
01	401-PHE	CZ	3.06
03	502-H_2O	01	3.40
N1	502-H2O	01	3.12
04	503-H_2O	01	3.20
C17	503-H2O	01	3.04
03	503-H_2O	01	2.27
C15	504-H2O	01	4.01
C17	504-H_2O	01	2.99
03	504-H2O	01	3.80
04	504-H_2O	01	1.78

Legend to Table 10. The table lists the interactions with IpBr2. The column headings are as follows:

#1 The atom of IpBr2 that interacts with the amino acid of the receptor. These are also numbered in figure 32.

#2 The amino acid in the full length rTRα that interacts with the ligand.

#3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.

#4 The distance in A between IpBr2 and the protein atom.

Table 11

T3 Atom	Amino Acid in full length α	Amino Acid Atom	Distance A
I2	215-PHE	CD1	4.08
I1	218-PHE	O	3.19
I1	218-PHE	CB	3.99
C4	218-PHE	CB	4.04
I1	218-PHE	C	3.79
I1	218-PHE	CB	3.99
I1	221-ILE	CG1	4.01
I1	222-ILE	CB	3.95
C8	222-ILE	CG1	3.91
C10	222-ILE	CD1	3.99
C12	222-ILE	CD1	3.57
C13	225-ALA	CD1	3.68
C3	225-ALA	CB	3.66
O4	228-ARG	CB	4.04
O4	228-ARG	NH1	3.23
C15	228-ARG	CZ	3.45
O3	228-ARG	NH2	3.54
O4	228-ARG	NH2	3.90
C10	256-MET	NH2	2.86
C12	256-MET	SD	3.73
C10	256-MET	SD	3.90
C12	256-MET	CE	3.97
I3	256-MET	CE	3.92
C11	259-MET	CE	3.89
C11	259-MET	C	3.95
C14	259-MET	O	3.59
N1	259-MET	O	3.51
C1	259-MET	O	3.88
C11	259-MET	CB	4.06
C13	259-MET	CB	3.77
C15	262-ARG	CB	3.96
C14	262-ARG	CB	3.61
O3	262-ARG	CB	4.02
O4	262-ARG	CB	3.65
O4	262-ARG	CB	3.92
N1	263-ALA	CD	3.72
N1	263-ALA	N	3.81
N1	263-ALA	CA	3.81
N1	275-THR	CB	3.63
N1	276-LEU	O	3.54
N1	276-LEU	CA	3.38
C5	276-LEU	C	3.73
C7	276-LEU	CD1	4.00
O2	276-LEU	CD1	4.05
C7	276-LEU	CD1	4.03
C9	276-LEU	CD2	3.80
C11	276-LEU	CD2	3.70
C14	277-SER	CD2	4.01
C15	277-SER	N	3.67
N1	277-SER	N	3.62
O3	277-SER	N	3.07
C15	277-SER	N	3.24
		CA	3.77

T3 Atom	Amino Acid in full length α	Amino Acid Atom	Distance A
O3	277-SER	CA	3.34
C13	277-SER	OG	3.92
I2	290-GLY	O	3.50
C4	292-LEU	CG	3.95
C8	292-LEU	CG	3.83
C2	292-LEU	CD1	4.07
C4	292-LEU	CD1	3.99
C4	292-LEU	CD2	4.09
C6	292-LEU	CD2	3.58
C8	292-LEU	CD2	3.50
C10	292-LEU	CD2	3.96
O1	292-LEU	CD2	3.71
I3	299-ILE	CD1	3.74
C8	381-HIS	CD2	3.94
C10	381-HIS	CD2	3.97
O1	381-HIS	CD2	3.39
O1	381-HIS	CD1	3.82
C8	381-HIS	NE2	3.47
C10	381-HIS	NE2	3.55
O1	381-HIS	NE2	2.70
O1	388-MET	CE	3.88
O1	401-PHE	CE1	3.52
O1	401-PHE	CZ	3.32
C14	502-H2O	O1	4.01
C15	502-H2O	O1	3.61
O3	502-H2O	O1	2.51
C15	503-H2O	O1	3.31
O4	503-H_2O	O1	3.10
N1	502-H_2O	O1	3.27
O3	503-H2O	O1	2.81
C15	504-H2O	O1	3.92
O4	504-H2O	O1	2.73

Legend to Table 11. The table lists the interactions with T3. The column headings are as follows:
#1 The atom of T3 that interacts with the amino acid of the receptor. These are also numbered in figure 32.
#2 The amino acid in the full length rTRα that interacts with the ligand.
#3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.
#4 The distance in A between T3 and the protein atom.

Table 12

Triac Atom	Amino Acid in full length hTR β	Amino Acid Atom	Distance A
I2	269-PHE	CD1	3.75
I2	269-PHE	CE1	3.88
I1	272-PHE	C	4.03
I1	272-PHE	O	3.54
I1	275-ILE	CG1	3.93
I1	276-ILE	CG1	4.02
C3	279-ALA	CB	3.81
C13	279-ALA	CB	3.87
C10	310-MET	SD	3.72
C12	310-MET	SD	3.78
C10	310-MET	CE	4.02
C12	310-MET	CE	3.92
I3	310-MET	CE	3.93
C13	313-MET	CA	3.94
C11	313-MET	C	3.72
C1	313-MET	O	3.79
C11	313-MET	O	3.12
C13	313-MET	O	3.55
C1	313-MET	CB	4.00
C11	313-MET	CB	3.82
C13	313-MET	CB	3.76
C13	313-MET	CG	3.88
O3	316-ARG	CB	3.99
O4	317-ALA	CA	4.08
O4	317-ALA	CA	4.10
C11	317-ALA	CB	3.70
I3	317-ALA	CB	4.10
O4	317-ALA	CB	4.06
O4	320-ARG	NH1	3.58
O3	320-ARG	NH2	3.55
O4	320-ARG	NH2	4.04
O4	329-THR	O	3.55
O4	330-LEU	CA	3.42
O4	330-LEU	C	3.77
C3	330-LEU	CB	4.06
C5	330-LEU	CB	4.08
C1	330-LEU	CD2	4.07
C3	330-LEU	CD2	4.00
C5	330-LEU	CD2	3.73
C7	330-LEU	CD2	3.51
C9	330-LEU	CD2	3.54
C11	330-LEU	CD2	3.86
C15	331-ASN	N	3.55
O3	331-ASN	N	3.74
O4	331-ASN	N	3.12
O3	331-ASN	CA	4.02
I2	344-GLY	O	3.87
C6	346-LEU	CD2	3.87
C8	346-LEU	CD2	3.84
O1	346-LEU	CD2	3.91
I3	353-ILE	CD1	3.51
C8	435-HIS	CD2	3.93
C10	435-HIS	CD2	3.79

Triac Atom	Amino Acid in full length hTR β	Amino Acid Atom	Distance A
O1	435-HIS	CD2	3.33
O1	435-HIS	CE1	3.81
C8	435-HIS	NE2	3.42
C10	435-HIS	NE2	3.33
O1	435-HIS	NE2	2.67
O1	442-MET	SD	3.96
O1	442-MET	CE	3.72
I2	442-MET	SD	4.01
O1	455-PHE	CE1	3.92
O1	455-PHE	CZ	3.50

Legend to Table 12. The table lists the interactions with Triac. The column headings are as follows:

#1 The atom of Triac that interacts with the amino acid of the receptor. These are also numbered in figure 32.

#2 The amino acid in the full length hTRβ that interacts with the ligand.

#3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.

#4 The distance in A between Triac and the protein atom.

DRAFT - 02/14/97

Table 13

GC1 Atom	Amino Acid in full length TR β	Amino Acid Atom	Distance A
C16	269-PHE	CE1	3.99
C19	272-PHE	O	3.85
C16	272-PHE	CB	3.98
C16	273-THR	CG2	3.76
C19	275-ILE	CG1	3.98
C19	276-ILE	CA	3.98
C2	276-ILE	CD1	3.88
C8	276-ILE	CD1	3.77
C10	276-ILE	CD1	3.58
C12	276-ILE	CD1	3.62
C19	276-ILE	CD1	3.56
C1	279-ALA	CB	3.68
C3	279-ALA	CB	3.56
O5	279-ALA	CB	3.11
O4	279-ALA	CB	3.90
O3	282-ARG	CZ	3.53
C17	282-ARG	NH1	3.87
O3	282-ARG	NH1	3.20
O4	282-ARG	NH1	3.85
C17	282-ARG	NH2	3.63
O3	282-ARG	NH2	3.00
C10	310-MET	SD	3.86
C12	310-MET	SD	3.91
C11	313-MET	C	3.85
C11	313-MET	O	3.41
C15	313-MET	O	3.87
C20	313-MET	O	3.99
C11	313-MET	CB	3.79
C1	313-MET	CG	3.94
C11	313-MET	CG	3.91
O5	313-MET	CG	3.87
O4	313-MET	CG	3.79
C20	314-SER	CA	4.00
C17	316-ARG	CB	3.95
C17	316-ARG	CD	3.80
O3	316-ARG	CD	3.83
O4	316-ARG	CD	3.51
C20	317-ALA	CB	3.93
C7	330-LEU	CD2	3.56
C9	330-LEU	CD2	3.63
C21	330-LEU	CD2	3.90
O5	331-ASN	N	3.62
C15	331-ASN	N	3.67
C18	344-GLY	O	3.60
C18	346-LEU	CG	3.89
C6	346-LEU	CD2	3.77
C8	346-LEU	CD2	3.80
C10	435-HIS	CD2	3.89
O1	435-HIS	CD2	3.64
O1	435-HIS	CE1	3.79
C8	435-HIS	NE2	3.44

GC1 Atom	Amino Acid in full length TR β	Amino Acid Atom	Distance A
C10	435-HIS	NE2	3.33
O1	435-HIS	NE2	2.77
O1	455-PHE	CE1	3.40
O1	455-PHE	CZ	3.22

Legend to Table 13. The table lists the interactions with GC1. The column headings are as follows:

#1 The atom of GC1 that interacts with the amino acid of the receptor. These are also numbered in figure 32.

#2 The amino acid in the full length hTRβ that interacts with the ligand.

#3 The name of the atom in the amino acid (standard nomenclature) where the interaction occurs.

#4 The distance in A between GC1 and the protein atom.

DOCKET ALARM

Table 14

Coordination Structure of TR-α and Dimit

Coordination Structure	R_1	R_2	R_3	R_5	R_6	R'_2	R'_3	R'_4	R'_5	R'_6	X
	$-CH_2-CH(NH_2)(CO_2)H$	-H	$-CH_3$	$-CH_3$	-H	-H	$-CH(CH_3)_2$	-OH	-H	-H	O
AA							215				
SS							H3				
AA			218				218				
SS			H3				H3				
AA							219				
SS							H3				
AA			221								
SS			H3								
AA							222	222	222	222	
SS							H3	H3	H3	H3	
AA	225										
SS	H3										
AA	228										
SS	H3										
AA									256	256	
SS									H5-H6	H5-H6	
AA	259				259						–
SS	H5-H6				H5-H6						
AA	262										
SS	H5-H6										
AA	263										
SS	H5-H6										
AA	266										
SS	loop										
AA	275										
SS	S3										
AA	276		276	276	276						
SS	S3		S3	S3	S3						
AA	277										
SS	loop										
AA							290-291				
SS							loop				
AA						292	292	292	292		292
SS						loop	loop	loop	loop		loop
AA				299							
SS				H8							
AA								381	381		
SS								H11	H11		
AA							388				
SS							H11				
AA							401	401			
SS							H12	H12			
AA	HOH5O2/HOH5O3/HOH5O4										
SS											

AA = Amino Acid SS = Secondary Structure

Table 15
Coordination Structure of TR-α and Triac

Coordination Structure	R_1 -	R_2	R_3	R_5	R_6	R'_2	R'_3	R'_4	R'_5	R'_6	X
	$-CH_2-COOH$	-H	-I	-I	-H	-H	-I	-OH	-H	-H	O
AA			218								
SS	-		H3								
AA			221								
SS			H3								
AA							222	222	222	222	
SS							H3	H3	H3	H3	
AA	225										
SS	H3										
AA				256					256	256	
SS				H5-H6					H5-H6	H5-H6	
AA	259				259						
SS	H5-H6				H5-H6						
AA	262										
SS	H5-H6										
AA	263										
SS	H5-H6										
AA	266										
SS	loop										
AA	275										
SS	S3										
AA	276		276	276	276						
SS	S3		S3	S3	S3						
AA	277										
SS	loop										
AA							290				
SS							loop				
AA						292	292	292	292		292
SS						loop	loop	loop	loop		loop
AA				299							
SS				H8							
AA								381	381		
SS								H11	H11		
AA								388			
SS								H11			
AA							401	401			
SS							H12	H12			

AA = Amino Acid SS = Secondary Structure

Table 16
Coordination Structure of TR-α and IpBr2

Coordination Structure	R_1	R_2	R_3	R_5	R_6	R'_2	R'_3	R'_4	R'_5	R'_6	X
	$-CH_2-CH(NH_2)(CO_2)H$	-H	-Br	-Br	-H	-H	$-CH(CH_3)_2$	-OH	-H	-H	O
AA							215				
SS							H3				
AA			218				218				
SS			H3				H3				
AA							219				
SS							H3				
AA			221								
SS			H3								
AA							222	222	222	222	
SS							H3	H3	H3	H3	
AA	225										
SS	H3										
AA	228										
SS	H3										
AA					256				256	256	
SS					H5-H6				H5-H6	H5-H6	
AA	259				259						
SS	H5-H6				H5-H6						
AA	262										
SS	H5-H6										
AA	263										
SS	H5-H6										
AA	266										
SS	loop										
AA	275										
SS	S3										
AA	276		276	276	276						
SS	S3		S3	S3	S3						
AA	277										
SS											
AA							290-291				
SS							loop				
AA						292	292	292	292		292
SS						loop	loop	loop	loop		loop
AA				299							
SS				H8							
AA								381	381		
SS								H11	H11		
AA							401	401			
SS							H12	H12			
AA	HOH5O2/HOH5O3/HOH5O4										
SS											

AA = Amino Acid SS = Secondary Structure

21376296
112497

Table 17

Coordination Structure of TR-α and Dimit

Coordination Structure	R_1	R_2	R_3	R_5	R_6	R'_2	R'_3	R'_4	R'_5	R'_6	X
	$-CH_2-CH(NH_2)(CO_2)H$	-H	-I	-I	-H	-H	-I	-OH	-H	-H	O
AA							215				
SS							H3				
AA			218			218					
SS			H3			H3					
AA			221								
SS			H3								
AA							222	222	222	222	
SS							H3	H3	H3	H3	
AA	225										
SS	H3										
AA	228										
SS	H3										
AA					256				256	256	
SS					H5-H6				H5-H6	H5-H6	
AA	259				259						
SS	H5-H6				H5-H6						
AA	262										
SS	H5-H6										
AA	263										
SS	H5-H6										
AA	275										
SS	S3										
AA	276		276	276	276						
SS	S3		S3	S3	S3						
AA	277										
SS											
AA							290				
SS							loop				
AA						292	292	292	292		292
SS						loop	loop	loop	loop		loop
AA				299							
SS				H8							
AA								381	381		
SS								H11	H11		
AA								388			
SS								H11			
AA							401	401			
SS							H12	H12			
AA	HOH502/HOH 503/HOH504										
SS											

AA = Amino Acid SS = Secondary Structure

Table 18

Coordination Structure of TR-β and Triac

Coordination Structure	R1	R2	R3	R5	R6	R2'	R3	R4	R5	R6	X
	$-CH_2CO_2H$	H	I	I	H	H	I	OH	H	H	O
AA							269				
SS							H3				
AA			272								
SS			H3								
AA			275								
SS			H3								
AA			276								
SS			H3								
AA	279	279									
SS	H3	H3									
AA				310					310	310	
SS				H5-H6					H5-H6	H5-H6	
AA	313				313						
SS	H5-H6				H5-H6						
AA	316										
SS	H5-H6										
AA	317				317		317				
SS	H5-H6				H5-H6		H5-H6				
AA	320										
SS	H5-H6										
AA	329										
SS	S3										
AA	330	330	330	330	330						
SS	S3	S3	S3	S3	S3						
AA	331										
SS	loop										
AA							344				
SS							loop				
AA							346	346			
SS							loop	loop			
AA				353							
SS				H8							
AA								435	435		
SS								H11	H11		
AA							442	442			
SS							H11	H11			
AA								455			
SS								H12			

AA = Amino Acid SS = Secondary Structure

Table 19

Coordination Structure of TR-β and GC1

Coordination Structure	R_1	R_2	R_3	R_5	R_6	R2	R3	R4	R5	R6	X
	$-O-CH_2CO_2H$	H	CH_3	CH_3	H	H	$CH(CH_3)$	OH	H	H	CH_2
AA							269				
SS							H3				
AA			272								
SS			H3								
AA			273				273				
SS			H3				H3				
AA			275								
SS			H3								
AA			276					276	276	276	
SS			H3					H3	H3	H3	
AA	279	279									
SS	H3	H3									
AA	282										
SS	H3										
AA				310					310	310	
SS				H5-H6					H5-H6	H5-H6	
AA	313				313						
SS	H5-H6				H5-H6						
AA							314				
SS							H5-H6				
AA	316										
SS	H5-H6										
AA							317				
SS							H5-H6				
AA	320										
SS	H5-H6										
AA	329										
SS	S3										
AA	330			330							
SS	S3			S3							
AA	331										
SS	loop										
AA							344				
SS							loop				
AA							346	346			
SS							loop	loop			
AA				353							
SS				H8							
AA								435	435		
								H11	H11		
								455			
SS								H12			

AA = Amino Acid SS = Secondary Structure